Neutrino-impact ionization of atoms in searches for neutrino magnetic moment

Konstantin A. Kouzakov

Department of Nuclear Physics and Quantum Theory of Collisions,

Faculty of Physics, Moscow State University, Moscow 119991, Russia[*]

Alexander I. Studenikin

Department of Theoretical Physics, Faculty of Physics,

Moscow State University, Moscow 119991, Russia[†]

Mikhail B. Voloshin

William I. Fine Theoretical Physics Institute,

University of Minnesota, Minneapolis, Minnesota 55455, USA

and Institute of Theoretical and Experimental Physics, Moscow, 117218, Russia[‡]

Abstract

The ionization of atomic electrons by scattering of neutrinos is revisited. This process is the one studied in the experimental searches for a neutrino magnetic moment using germanium detectors. Current experiments are sensitive to the ionization energy comparable with the atomic energies, and the effects of the electron binding should be taken into account. We find that the so-called stepping approximation to the neutrino-impact ionization is in fact exact in the semiclassical limit and also that the deviations from this approximation are very small already for the lowest bound Coulomb states. We also consider the effects of electron-electron correlations and argue that the resulting corrections to the ionization of independent electrons are quite small. In particular we estimate that in germanium these are at a one percent level at the energy transfer down to a fraction of keV. Exact sum rules are also presented as well as analytical results for a few lowest hydrogen-like states.

[*]Electronic address: kouzakov@srd.sinp.msu.ru

[†]Electronic address: studenik@srd.sinp.msu.ru

[‡]Electronic address: voloshin@umn.edu

I. INTRODUCTION

The neutrino magnetic moments (NMM) expected in the Standard Model are very small and proportional to the neutrino masses [1]: $\mu_\nu \approx 3 \times 10^{-19} \, \mu_B \, (m_\nu/1 \, eV)$ with $\mu_B = e/2m$ being the electron Bohr magneton, and m is the electron mass. Thus any larger value of μ_ν can arise only from physics beyond the Standard Model (a recent review of this subject can be found in Ref. [2]). Current direct experimental searches [3–5] for a magnetic moment of the electron (anti)neutrinos from reactors have lowered the upper limit on μ_ν down to $\mu_\nu < 3.2 \times 10^{-11} \, \mu_B$ [5]. These ultra low background experiments use germanium crystal detectors exposed to the neutrino flux from a reactor and search for scattering events by measuring the energy T deposited by the neutrino scattering in the detector. The sensitivity of such a search to NMM crucially depends on lowering the threshold for the energy transfer T, due to the enhancement of the magnetic scattering relative to the standard electroweak one at low T. Namely, the differential cross section $d\sigma/dT$ is given by the incoherent sum of the magnetic and the standard cross section, and for the scattering on free electrons the NMM contribution is given by the formula [6, 7]

$$\frac{d\sigma_{(\mu)}}{dT} = 4\pi \, \alpha \, \mu_\nu^2 \left(\frac{1}{T} - \frac{1}{E_\nu} \right) = \pi \, \frac{\alpha^2}{m^2} \left(\frac{\mu_\nu}{\mu_B} \right)^2 \left(\frac{1}{T} - \frac{1}{E_\nu} \right) \tag{1}$$

where E_ν is the energy of the incident neutrino, and displays a $1/T$ enhancement at low energy transfer. The standard electroweak contribution is constant in T at $E_\nu \gg T$:

$$\frac{d\sigma_{EW}}{dT} = \frac{G_F^2 \, m}{2\pi} \left(1 + 4 \sin^2 \theta_W + 8 \sin^4 \theta_W \right) \left[1 + O\left(\frac{T}{E_\nu} \right) \right] \approx 5 \times 10^{-48} \, \text{cm}^2/\text{keV}. \tag{2}$$

In what follows we refer to these two types of contribution to the scattering as, respectively, the magnetic and the weak.

The current experiments have reached threshold values of T as low as few keV and are likely to further improve the sensitivity to low energy deposition in the detector. At low energies however one can expect a modification of the free-electron formulas (1) and (2) due to the binding of electrons in the germanium atoms, where e.g. the energy of the K_α line, 9.89 keV, indicates that at least some of the atomic binding energies are comparable to the already relevant to the experiment values of T. Thus a proper treatment of the atomic effects in neutrino scattering is necessary and important for the analysis of the current and even more of the future data with a still lower threshold. Furthermore, there is no

known means of independently calibrating experimentally the response of atomic systems, such as the germanium, to the scattering due to the interactions relevant for the neutrino experiments. Therefore one has to rely on a pure theoretical analysis in interpreting the neutrino data. This problem had been addressed numerically in the past [8, 9] and the interest to the problem was renewed in several recent papers, which however are ridden by a 'trial and error' approach. The early claim [10] of a significant enhancement of the NMM contribution by the atomic effects has been later disproved [11, 12] and it was argued [11] that the modification of the formulas (1) and (2) by the atomic binding effects is insignificant down to very low values of T. It has been subsequently pointed out [13] that the analysis of Ref. [11] is generally invalidated in multi-electron systems, including atoms with $Z > 1$. Furthermore, the analysis of Ref. [11] is also generally invalidated by singularities of the relevant correlation function in the complex plane of momentum transfer, so that the claimed behavior of the cross section at low T applies only in the semiclassical limit, although, as will be shown here, it gives a very good approximation to the actual behavior for an electron bound by a Coulomb potential.

In this paper we revisit the subject of neutrino scattering on atoms at low energy transfer. We aim at describing this process at T in the range of few keV and lower, so that the motion of the electrons is considered as strictly nonrelativistic. Also in this range the energy of the dominant part of the incident neutrinos from the reactor is much larger than T and we thus neglect any terms whose relative value is proportional to T/E_ν (in particular, in this range one can neglect the $1/E_\nu$ term in Eq.(1) in comparison with $1/T$). Furthermore any recoil of the germanium atom as a whole results in an energy transfer less than $2E_\nu^2/M_{Ge}$, which at the typical reactor neutrino energy is well below the considered here keV range of the energy transfer. Thus we formally set the mass of the atomic nucleus to infinity and neglect any recoil by the atom as a whole. In particular, under these conditions the interaction of the neutrino with the nucleus can be entirely neglected, and only the scattering on the atomic electrons is to be considered.

We find that in the scattering on realistic atoms, such as germanium, the so-called stepping approximation works with a very good accuracy. The stepping approach, introduced in Ref. [8] from an interpretation of numerical data, treats the process as scattering on individual independent electrons occupying atomic orbitals and suggests that the cross section follows the free-electron behavior in Eqs.(1) and (2) down to T equal to the ionization

3

threshold for the orbital, and that below that energy the electron on the corresponding orbital is 'deactivated' thus producing a sharp 'step' in the dependence of the cross section on T. In the present paper, we consider general relations for the discussed scattering on atomic systems in Sec. II and present in Appendix A sum rules for the theoretical objects involved in the calculations [18]. In Sec. III we prove that for the scattering on individual electrons the stepping approximation becomes exact in the semiclassical limit, so that its applicability is improved with the principal number n of the atomic orbital. We also find by an explicit calculation (Appendix B) for a hydrogen-like ground state, i.e. at $n = 1$, that the deviation from the stepping behavior is less than 5% at the worst point, where the energy transfer T is exactly at the threshold. The accuracy of the approach based on considering the scattering on individual electrons is limited by the existence of the electron-electron correlations in the process. We consider the correction introduced by these correlations in Sec. IV and, in Sec. V, apply the derived formula to an estimate of the effect for germanium, using the Thomas-Fermi model. We find that the correlation correction grows at smaller T but is still small, of order of a few percent, for T in the range of a few hundred eV. We thus argue that the stepping approach describes the scattering cross section with a sufficient for practical purposes accuracy, and that it can be applied to the analysis of the present and future data of searches for NMM with germanium detectors down to the values of the energy deposition $T \sim 0.3 \, \text{keV}$.

II. GENERAL FORMULAS FOR NEUTRINO SCATTERING ON ATOMIC ELECTRONS

In this section we briefly recapitulate the general expressions and introduce the relevant atomic objects for the neutrino scattering on atomic electrons. We start with the magnetic process and then also apply a similar treatment to the standard weak part of the cross section.

The kinematics of the scattering of a neutrino on atomic electrons is generally characterized by the components of the four-momentum transfer, the energy transfer T and the spatial momentum transfer $\vec{q}$, from the neutrino to the electrons with two rotationally invariant variables being T and $q^2 = \vec{q}^{\,2}$. At small T the electrons can be treated nonrelativistically both in the initial and the final state, so that the process is that of scattering of

an NMM in the electromagnetic field $A = (A_0, \vec{A})$ of the electrons: $A_0(\vec{q}) = \sqrt{4\pi\alpha}\,\rho(\vec{q})/\vec{q}^2$, $\vec{A}(\vec{q}) = \sqrt{4\pi\alpha}\,\vec{j}(\vec{q})/\vec{q}^2$, where $\rho(\vec{q})$ and $\vec{j}(\vec{q})$ are the Fourier transforms of the electron number density and current density operators, respectively,

$$\rho(\vec{q}) = \sum_{a=1}^{Z} \exp(i\vec{q}\cdot\vec{r}_a) \;, \tag{3}$$

$$\vec{j}(\vec{q}) = -\frac{i}{2m}\sum_{a=1}^{Z}\left[\exp(i\vec{q}\cdot\vec{r}_a)\frac{\partial}{\partial\vec{r}_a} + \frac{\partial}{\partial\vec{r}_a}\exp(i\vec{q}\cdot\vec{r}_a)\right]\;, \tag{4}$$

and the sums run over the positions $\vec{r}_a$ of all the Z electrons in the atom.

In this limit the expression for the double differential cross section is given by [13]

$$\frac{d^2\sigma_{(\mu)}}{dT\,dq^2} = 4\pi\,\alpha\,\frac{\mu_\nu^2}{q^2}\left[\left(1 - \frac{T^2}{q^2}\right)S(T,q^2) + \left(1 - \frac{q^2}{4E_\nu^2}\right)R(T,q^2)\right]\;, \tag{5}$$

where $S(T,q^2)$, also known as the dynamical structure factor [15], and $R(T,q^2)$ are

$$S(T,q^2) = \sum_n \delta(T - E_n + E_0)\,|\langle n|\rho(\vec{q})|0\rangle|^2\,, \tag{6}$$

$$R(T,q^2) = \sum_n \delta(T - E_n + E_0)\,|\langle n|j_\perp(\vec{q})|0\rangle|^2\,, \tag{7}$$

with $j_\perp$ being the $\vec{j}$ component perpendicular to $\vec{q}$ and parallel to the scattering plane, which is formed by the incident and final neutrino momenta. The sums in Eqs. (6) and (7) run over all the states $|n\rangle$ with energies E_n of the electron system, with $|0\rangle$ being the initial state.

Clearly, the factors $S(T,q^2)$ and $R(T,q^2)$ are related to respectively the density-density and current-current Green's functions

$$F(T,q^2) = \sum_n \frac{|\langle n|\rho(\vec{q})|0\rangle|^2}{T - E_n + E_0 - i\,\epsilon} = \left\langle 0\left|\rho(-\vec{q})\,\frac{1}{T - H + E_0 - i\,\epsilon}\,\rho(\vec{q})\right|0\right\rangle\,, \tag{8}$$

$$L(T,q^2) = \sum_n \frac{|\langle n|j_\perp(\vec{q})|0\rangle|^2}{T - E_n + E_0 - i\,\epsilon} = \left\langle 0\left|j_\perp(-\vec{q})\,\frac{1}{T - H + E_0 - i\,\epsilon}\,j_\perp(\vec{q})\right|0\right\rangle\,, \tag{9}$$

as

$$S(T,q^2) = \frac{1}{\pi}\,\mathrm{Im}F(T,q^2)\,, \tag{10}$$

$$R(T,q^2) = \frac{1}{\pi}\,\mathrm{Im}L(T,q^2)\,, \tag{11}$$

5

with H being the Hamiltonian for the system of electrons. For small values of q, in particular, such that $q \sim T$, only the lowest-order non-zero terms of the expansion of Eqs. (10) and (11) in powers of q^2 are of relevance (the so-called dipole approximation). In this case, one has [13]

$$R(T, q^2) = \frac{T^2}{q^2} S(T, q^2). \tag{12}$$

Taking into account Eq. (12), the experimentally measured singe-differential inclusive cross section is, to a good approximation, given by (see e.g. in Refs. [11, 13])

$$\frac{d\sigma_{(\mu)}}{dT} = 4\pi \, \alpha \, \mu_\nu^2 \int_{T^2}^{4E_\nu^2} S(T, q^2) \frac{dq^2}{q^2} \, . \tag{13}$$

The standard electroweak contribution to the cross section can be similarly expressed in terms of the same factor $S(T, q^2)$ [11] as

$$\frac{d\sigma_{EW}}{dT} = \frac{G_F^2}{4\pi} \left(1 + 4 \sin^2 \theta_W + 8 \sin^4 \theta_W \right) \int_{T^2}^{4E_\nu^2} S(T, q^2) \, dq^2 \, , \, , \tag{14}$$

where the factor $S(T, q^2)$ is integrated over q^2 with a unit weight, rather than q^{-2} as in Eq.(13).

The kinematical limits for q^2 in an actual neutrino scattering are explicitly indicated in Eqs.(13) and (14). At large E_ν, typical for the reactor neutrinos, the upper limit can in fact be extended to infinity, since in the discussed here nonrelativistic limit the range of momenta $\sim E_\nu$ is indistinguishable from infinity. The lower limit can be shifted to $q^2 = 0$, since the contribution of the region of $q^2 < T^2$ can be expressed in terms of the photoelectric cross section [11] and is negligibly small (at the level of below one percent in the considered range of T). For this reason we henceforth discuss the momentum-transfer integrals in Eqs. (13) and (14) running from $q^2 = 0$ to $q^2 = \infty$:

$$I_1(T) = \int_0^\infty S(T, q^2) \frac{dq^2}{q^2} \, , \qquad \text{and} \qquad I_2(T) = \int_0^\infty S(T, q^2) \, dq^2 \, . \tag{15}$$

For a free electron, which is initially at rest, the density-density correlator is the free particle Green's function

$$F_{(FE)}(T, q^2) = \left(T - \frac{q^2}{2m} - i\,\epsilon \right)^{-1} \tag{16}$$

so that the dynamical structure factor is given by $S_{(FE)}(T, q^2) = \delta(T - q^2/2m)$, and the discussed here integrals are in the free-electron limit as follows:

$$I_1^{(FE)} = \int_0^\infty S_{(FE)}(T, q^2) \frac{dq^2}{q^2} = \frac{1}{T} \, , \qquad I_2^{(FE)} = \int_0^\infty S_{(FE)}(T, q^2) \, dq^2 = 2\,m \, . \tag{17}$$

6

Clearly, these expressions, when used in the formulas (13) and (14), result in the free-electron cross section in Eqs. (1) and (2).

III.   SCATTERING ON ONE BOUND ELECTRON

The binding effects generally deform the density-density Green's function, so that both the integrals (15) are somewhat modified. Namely, the binding effects spread the free-electron δ-peak in the dynamical structure function at $q^2 = 2mT$ and also shift it by the scale of characteristic electron momenta in the bound state. However it turns out that the free electron expressions are quite robust in the sense that in realistic systems the modification of the integrals relative to their free-electron limit, are quite small. As a formal statement, we will show in the Appendix A that when the function $F(T, q^2)$ is analytically continued in complex plane of q^2 the free-electron expressions are valid for the integrals over q^2 extending from $-\infty$ to $+\infty$, and in the case of the integral, similar to I_2 i.e. with the weight q^0, this property also holds for scattering on multi-electron atomic systems, while for that with the weight q^{-2} it generally holds only for the scattering on one electron, or on independent electrons. Clearly the latter integrals over the full axis of q^2 differ from those of physical interest in Eq.(15) by the contribution of negative q^2, which although numerically small even at low T, still makes the scattering on bound electrons different from that on free electrons.

In this section we consider the scattering on just one electron. The Hamiltonian for the electron has the form $H = p^2/2m + V(r)$, and the density-density Green's function from Eq.(8) can be written as

$$
\begin{aligned}
F(T, q^2) &= \left\langle 0 \left| e^{-i\vec{q}\cdot\vec{r}} \left[T - H(\vec{p}, \vec{r}) + E_0 \right]^{-1} e^{i\vec{q}\cdot\vec{r}} \right| 0 \right\rangle \\
&= \left\langle 0 \left| \left[T - H(\vec{p} + \vec{q}, \vec{r}) + E_0 \right]^{-1} \right| 0 \right\rangle \\
&= \left\langle 0 \left| \left[T - \frac{\vec{q}^2}{2m} - \frac{\vec{p}\cdot\vec{q}}{m} - H(\vec{p}, \vec{r}) + E_0 \right]^{-1} \right| 0 \right\rangle ,
\end{aligned} \tag{18}
$$

where the infinitesimal shift $T \to T - i\epsilon$ is implied.

Clearly, a nontrivial behavior of the latter expression in Eq.(18) is generated by the presence of the operator $(\vec{p}\cdot\vec{q})$ in the denominator, and the fact that it does not commute with the Hamiltonian H. Thus an analytical calculation of the Green's function as well as the dynamical structure factor is feasible in only few specific problems. In Appendix B

7

we present such a calculation for ionization from the $1s$, $2s$ and $2p$ hydrogen-like states. In particular, we find that the deviation of the discussed integrals (15) from their free values are very small: the largest deviation is exactly at the ionization threshold, where, for instance, each of the $1s$ integrals is equal to the free-electron value multiplied by the factor $(1 - 7\,e^{-4}/3) \approx 0.957$ [19].

The problem of calculating the integrals (15) however can be solved in the semiclassical limit, where one can neglect the noncommutativity of the momentum $\vec{p}$ with the Hamiltonian, and rather treat this operator as a number vector. Taking also into account that $(H - E_0)\,|0\rangle = 0$, one can then readily average the latter expression in Eq.(18) over the directions of $\vec{q}$ and find the formula for the dynamical structure factor:

$$S(T, q^2) = \frac{m}{2\,p\,q}\left[\theta\left(T - \frac{q^2}{2m} + \frac{p\,q}{m}\right) - \theta\left(T - \frac{q^2}{2m} - \frac{p\,q}{m}\right)\right]\,, \tag{19}$$

where $p = |\vec{p}|$ and θ is the standard Heaviside step function. The expression in Eq.(19) is nonzero only in the range of q satisfying the condition $-p\,q/m < T - q^2/2m < p\,q/m$, i.e. between the (positive) roots of the binomials in the arguments of the step functions: $q_{min} = \sqrt{2m\,T + p^2} - p$ and $q_{max} = \sqrt{2m\,T + p^2} + p$. One can notice that the previously mentioned 'spread and shift' of the peak in the dynamical structure function in this limit corresponds to a flat pedestal between q_{min} and q_{max}. The calculation of the integrals (15) with the expression (19) is straightforward, and yields the free-electron expressions (17) for the discussed here integrals in the semiclassical (WKB) limit [20]:

$$I_1^{(WKB)} = \frac{1}{T}\,, \qquad I_2^{(WKB)} = 2\,m\,. \tag{20}$$

The difference from the pure free-electron case however is in the range of the energy transfer T. Namely, the expressions (20) are applicable in this case only above the ionization threshold, i.e. at $T \geq |E_0|$. Below the threshold the electron becomes 'inactive'.

It is instructive to point out that the validity of the result in Eq.(20) is based on the semiclassical approximation and is not directly related to the value of the energy T. In particular, for a Coulomb interaction the WKB approximation is applicable at energy near the threshold [14]. For T exactly at the threshold, $T = -E_0$, the criterion for applicability of the semiclassical approach in terms of the force $F = |\vec{F}| = |[\vec{p}, H]|$ acting on the electron and the momentum p of the electron is that [14] the ratio of the characteristic values mF/p^3 is small. For the excitation of a state with the principal number n this ratio behaves parametrically as $1/n$ [21]. Thus the applicability of a semiclassical treatment of the ionization

near the threshold improves for initial states with large n. As previously mentioned, the modification of the integrals (15) by the binding is already less than 5% for $n = 1$, so that we fully expect this deviation to be smaller for the higher states, and even smaller at larger values of T above the threshold due to the approach to the free-electron behavior at $T \gg E_0$.

We believe that the latter conclusion explains the so-called stepping behavior observed empirically [8] in the results of numerical calculations. Namely the calculated cross section $d\sigma/dT$ for ionization of an electron from an atomic orbital follows the free-electron dependence on T all the way down to the threshold for the corresponding orbital with a very small, at most a few percent, deviation. This observation lead the authors of Ref. [8] to suggest the stepping approximation for the ratio of the atomic cross section (per target electron) to the free-electron one:

$$f(T) \equiv \frac{d\sigma/dT}{(d\sigma/dT)_{FE}} = \frac{1}{Z} \sum_i n_i \, \theta(T - |E_i|) \; , \tag{21}$$

where the sum runs over the atomic orbitals with the binding energies E_i and the filling numbers n_i. Clearly, the factor $f(T)$ simply counts the fraction of 'active' electrons at the energy T, i.e. those for which the ionization is kinematically possible. For this reason we refer to $f(t)$ as an *activation factor*. We conclude here that the stepping approximation is indeed justified with a high accuracy in the approximation of the scattering on independent electrons, i.e. if one neglects the two-electron correlations induced by the interference of terms in the operator $\rho(\vec{q})$ in Eq.(3) corresponding to different electrons. In the next section we estimate the effect of such an interference and find that the resulting corrections are small, at least in atoms with large Z, such as the germanium.

IV. TWO-ELECTRON CORRELATION

In this section we discuss the correction arising from a correlation between two electrons. We consider the energy T and hence the relevant momentum transfer q as large in comparison with the atomic scale. In this way we estimate the relevant parameter for the significance of the correlation effect.

We start with consider an isolated system of two electrons interacting among themselves through the Coulomb potential $V(r)$. The Hamiltonian for this system thus has the form

$$H = \frac{P^2}{4m} + \frac{p^2}{m} + V(r) \; , \tag{22}$$

9

where $\vec{P} = -i\partial/\partial\vec{R}$ and $\vec{p} = -i\partial/\partial\vec{r}$ are, as usual, the momenta conjugate to respectively the center of mass coordinate $\vec{R}$ and the relative coordinate $\vec{r}$.

The spatial part of the wave function of the system factorizes into the product $\phi(\vec{R})\,\psi(\vec{r})$ with $\phi(\vec{R})$ while the spin part will be considered later. We consider here the system at rest, i.e. $\phi(R) = \text{const}$, since a boost to a momentum P does not change the cross section.

The density-density Green's function then takes the form

$$F(T, q^2) = \sum_n \frac{\langle 0 \left| e^{i\vec{q}\vec{r}/2} + e^{-i\vec{q}\vec{r}/2} \right| n \rangle \langle n \left| e^{i\vec{q}\vec{r}/2} + e^{-i\vec{q}\vec{r}/2} \right| 0 \rangle}{T - \frac{q^2}{4m} - E_n + E_0} \; , \qquad (23)$$

where the states $|0\rangle$, $|n\rangle$ and the energies E_0, E_n refer to the relative motion in the system with $|0\rangle$ standing for the initial state. Clearly, it is implied in Eq.(23) that the corresponding matrix elements for the (trivial) dynamics of the system as a whole are already taken, which results in replacing in the energy denominator the excitation energy T by its value corrected for the recoil of the system as a whole: $T \to T - q^2/4m$.

The cross terms between $\exp(i\vec{q}\cdot\vec{r}/2)$ and $\exp(-i\vec{q}\cdot\vec{r}/2)$ in the expression (23) result in the previously discussed one-particle Green's function

$$F_1(T, q^2) = 2 \left\langle 0 \left| \left(T - \frac{q^2}{2m} - \frac{\vec{p}\cdot\vec{q}}{m} - H + E_0 \right)^{-1} \right| 0 \right\rangle \; , \qquad (24)$$

where the overall factor of 2 arises from the two identical (after averaging over the direction of $\vec{q}$) cross terms, and physically is corresponding to the presence of two particles in the system.

The discussed here contribution of the two-electron correlation arises from the diagonal terms, whose contribution is given by

$$F_c(T, q^2) = 2\,\eta \sum_n \frac{\langle 0 \left| e^{i\vec{q}\vec{r}/2} \right| n \rangle \langle n \left| e^{i\vec{q}\vec{r}/2} \right| 0 \rangle}{T - \frac{q^2}{4m} - E_n + E_0} \; , \qquad (25)$$

where, again, the two terms give the same contribution after the averaging over the direction of $\vec{q}$, which is accounted for by the factor of 2 in the latter expression. The factor η is the symmetry factor for the spin part of the two-electron system: $\eta = -1$ for the spin-singlet state of the pair and $\eta = +1$ for the spin-triplet. The appearance of this factor can be explained as follows. The discussed correlation arises from the situation where an excitation of one electron by the operator ρ produces the same spatial wave function as an excitation of another one. In order for the wave functions to be identical the spin variables of the

two electrons should also be switched, which operation results in the factor η. Clearly, no such factor arises in the one-particle term (24) since the spin of both electrons simply 'goes through'. It can be also mentioned that, naturally, the symmetry of the spatial wave function $\psi(\vec{r})$ is opposite to η.

One can notice that unlike in the one-particle contribution (Eq.(24)) where the momentum $\vec{q}$ flows in and out of the system, the correlation contribution in Eq.(25) corresponds to the net momentum $\vec{q}$ flowing into the system. Clearly, for non-interacting particles such contribution would vanish and the whole correlation effect arises only due to the interaction between the electrons, which interaction absorbs the momentum transfer. The term (25) can be graphically represented as shown in Fig.1, where the system lines correspond to the propagation of the system in the potential V with the outer legs corresponding to the wave functions of the initial state in the momentum space $\langle\psi(\vec{p}')|$ and $|\psi(\vec{p})\rangle$ and the line between the action of the operators $\exp(i\vec{q}\cdot\vec{r}/2)$ corresponding to the Green's function. One can write in terms of these objects the expression for $F_c(T, q^2)$ as

$$F_c(T, q^2) = 2 \int \frac{d^3 p'}{(2\pi)^3} \int \frac{d^3 p}{(2\pi)^3} \, \psi^*(\vec{p}') \, G(E; \vec{p}' - \frac{\vec{q}}{2}, \vec{p} + \frac{\vec{q}}{2}) \, \psi(\vec{p}) \ , \qquad (26)$$

where $G(E, \vec{k}', \vec{k})$ is the Green's function $(E - H)^{-1}$ in the momentum representation at the energy $E = T + E_0 - q^2/4m$.

We shall consider separately the effect of the interaction in the wave functions and in the
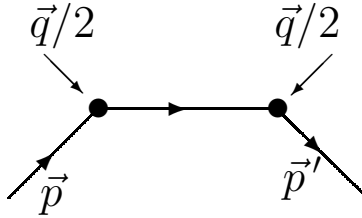

FIG. 1: Graphical representation of the two-electron correlation. The external legs correspond to the momentum-space wave function and the propagator is the Green's function in the potential V.

Green's function. For the zeroth order Green's function

$$G_0(E, \vec{k}', \vec{k}) = \frac{(2\pi)^3 \, \delta^{(3)}(\vec{k}' - \vec{k})}{E - k^2/m} \qquad (27)$$

and the exact wave functions one finds

$$F_c^{(0)}(T, q^2) = 2\,\eta \int \frac{d^3p}{(2\pi)^3} \frac{\psi^*(\vec{p}+\vec{q})\,\psi(\vec{p})}{T - \frac{q^2}{2m} - \frac{(\vec{p}\cdot\vec{q})}{m} - \frac{p^2}{m} + E_0}\,. \tag{28}$$

Let us consider now q as a large parameter in comparison with the characteristic momenta p_0 in $\psi(\vec{p})$, beyond which the wave function falls off. At such values of q the product $\psi^*(\vec{p}+\vec{q})\,\psi(\vec{p})$ carries a suppression in only one of the factors in two regions of $\vec{p}$: one where $p \sim p_0$ and the other where $|\vec{p}+\vec{q}| \sim p_0$. Clearly, by shifting the integration variable $\vec{p}+\vec{q} \to \vec{p}$ one can readily see that both integration regions the contribution of the latter region is the same as of the first one, so that one evaluates the integral in Eq.(28) by considering only the contribution of the region $p \ll q$ and taking it with a factor of two. Then the leading at large q expression for the function in Eq.(28) takes the form

$$F_c^{(0)}(T, q^2) = 4\,\eta\, \frac{\psi^*(\vec{q})}{T - \frac{q^2}{2m}} \int \frac{d^3p}{(2\pi)^3}\, \psi(\vec{p}) = 4\,\eta\, \frac{\psi^*(\vec{q})\,\psi(0)}{T - \frac{q^2}{2m}}\,, \tag{29}$$

The appearance of the wave function at the origin $\vec{r} = 0$, $\psi(0)$, in this expression implies that at large q the considered contribution to the correlation arises only for an S-wave relative motion within the electron pair, which thus have to be a spin-singlet, and therefore $\eta = -1$.

In fact for an for an S-wave motion the momentum-space wave function $\psi(\vec{q})$ can be also expressed at large q in terms of the position-space wave function at the origin $\psi(0)$. Indeed, in the S-wave the wave function is a function of r: $\psi(r)$. At small r the Coulomb repulsion between the electrons dominates over all other interactions and the Schrödinger equation for $\psi(r)$ reads

$$-\frac{1}{m}\,\psi'' - \frac{2}{m\,r}\,\psi'(r) + \frac{\alpha}{r}\,\psi(r) = E\,\psi(r)\,. \tag{30}$$

By requiring the two singular at $r \to 0$ as $1/r$ terms to match in this expression, one finds that the derivative of $\psi(r)$ over r at the origin is expressed in terms of $\psi(0)$:

$$\psi'(0) = \frac{m\,\alpha}{2}\,\psi(0)\,. \tag{31}$$

A finite derivative over r implies that the gradient $\vec{\nabla}\psi(r) = \vec{r}\psi'(r)/r$ is singular at $r = 0$, so that the asymptotic at large $|\vec{q}|$ behavior of the momentum space wave function is proportional to $1/|\vec{q}|^4$ with the coefficient determined by $\psi'(0)$, which in turn is determined, according to Eq.(31), by $\psi(0)$:

$$\psi(\vec{q})|_{|\vec{q}|\to\infty} = -\frac{4\pi\,m\,\alpha\,\psi(0)}{|\vec{q}|^4}\,. \tag{32}$$

12

Using this relation in Eq.(29) one finds in the large q^2 limit

$$F_c^{(0)}(T, q^2) = 16\,\pi\,\alpha\,\frac{m\,|\psi(0)|^2}{q^4}\,\frac{1}{T - \frac{q^2}{2m}}\,.\tag{33}$$

The latter expression is manifestly proportional to first power of the interaction between the electrons. Therefore a similar contribution can arise from the first order in the expansion of the Green's function in the interaction potential V. In this order one finds for the discussed correlation part of $F(T, q^2)$:

$$F_c^{(1)}(T, q^2) = 2\eta \int \frac{d^3p'}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \frac{\psi^*(\vec{p}')\,V(-\vec{q}+\vec{p}'-\vec{p})\,\psi(\vec{p})}{\left[T - \frac{q^2}{2m} + \frac{(\vec{p}'\cdot\vec{q})}{m} - \frac{p'^2}{m} + E_0\right]\left[T - \frac{q^2}{2m} - \frac{(\vec{p}\cdot\vec{q})}{m} - \frac{p^2}{m} + E_0\right]}\,,\tag{34}$$

where $V(\vec{k})$ is the Fourier transform of the potential, so that for the Coulomb repulsion between the electrons

$$V(\vec{k}) = \frac{4\pi\alpha}{k^2}.\tag{35}$$

Considering as before the limit of large q and thus neglecting p and p' in comparison with q, one readily finds that the result is again proportional to $|\psi(0)|^2$, so that the effect remains only in the S-wave (and hence $\eta = -1$):

$$F_c^{(1)}(T, q^2)\big|_{mT, q^2 \gg p^2, p'^2} = -8\pi\,\alpha\,\frac{|\psi(0)|^2}{q^2\left(T - \frac{q^2}{2m}\right)^2}\tag{36}$$

Collecting the formulas (33) and (36) together one finds the estimate of the two-electron correlation part of $F(T, q^2)$ in the limit of large T and q^2:

$$F_c(T, q^2) = 8\pi\,\alpha\,|\psi(0)|^2\left[\frac{2\,m}{q^4\left(T - \frac{q^2}{2m}\right)} - \frac{1}{q^2\left(T - \frac{q^2}{2m}\right)^2}\right]\,.\tag{37}$$

The corresponding two-electron correlation correction to the integrals for the neutrino scattering cross section, is then calculated by shifting $T \to T - i\epsilon$ and considering only the contribution of the singularity at $q^2 = 2m\,T$:

$$\frac{1}{\pi}\int \mathrm{Im}F_c(T, q^2)\,\frac{dq^2}{q^2} = -4\pi\,\alpha\,\frac{|\psi(0)|^2}{m\,T^3}\,,\qquad \frac{1}{\pi}\int \mathrm{Im}F_c(T, q^2)\,dq^2 = 0\,.\tag{38}$$

Notice, that the two-electron contribution to the integral relevant for the standard electroweak scattering vanishes in the discussed approximation due to a cancellation of the two terms in Eq.(37).

The discussed here calculation shows, as expected, that at large q the two-electron correlation arises only when the electrons are separated by a short distance. For this reason one can relax the assumption, we made in the beginning of this section, that the system of two electrons is in a free motion. Indeed the same result would apply in the situation, where the pair as a whole moves in a potential that is sufficiently smooth so that the 'tidal force' interaction with the rest of the atomic system does not overcome the Coulomb singularity of the repulsion between the electrons at distances of order $1/q$.

V.   SCATTERING ON ATOMIC ELECTRONS IN GERMANIUM

In considering the neutrino scattering on actual atoms one needs to evaluate the dependence of the number of active electrons on T and generally also evaluate the effect of the two-electron correlations. The energies of the inner K, L and M orbitals in the germanium atom are well known (see e.g. Ref. [9] and references therein) and provide the necessary data for a description of the neutrino scattering by the stepping formula (21) down to the values of the energy transfer T in the range of the binding of the M electrons, i.e. at $T > |E_M| \approx 0.18\,\text{keV}$. The corresponding steps in the activation factor are shown in Fig. 2. It can be mentioned that if one applies formulas of the Appendix B to the onset of the K shell step, i.e. just above $10.9\,\text{keV}$, the difference from the shown in the plot step function would be practically invisible in the scale of Fig. 2.

Our goal in this section is to estimate the effect of the two-electron correlations in the scattering on germanium. We shall estimate this effect by considering the atomic number Z as a large parameter and using the Thomas-Fermi model, which, in spite of its known shortcomings, appears to be appropriate for evaluating average bulk properties of atomic electrons at large Z, such as in the problem at hand.

In the Thomas-Fermi model (see e.g. Ref. [14]) the atomic electrons are described as a degenerate free electron gas in a master potential $\phi(r)$ filling the momentum space up to the zero Fermi energy, i.e. up to the momentum $p_0(r)$ such that $p_0^2/2m - e\phi = 0$. The electron density $n(r) = p_0^3/(3\pi^2)$ then determines the potential $\phi(r)$ from the usual Gauss equation. In the discussed picture at an energy transfer T the ionization is possible only for the electrons whose energies in the potential are above $-T$, i.e. with momenta above $p_T(r)$ with $p_T^2/2m - e\phi = -T$. The electrons with lower energy are inactive. Calculating

the density of the inactive electrons as $p_T^3/(3\pi^2)$ and subtracting their total number from Z, one readily arrives at the formula for the activation factor, i.e. the effective fraction of the active electrons Z_{eff}/Z as a function of T:

$$f(T) = \frac{Z_{\text{eff}}(T)}{Z} = 1 - \int_0^{x(T)} \left[\frac{\chi(x)}{x} - \frac{T}{T_0}\right]^{3/2} x^2 \, dx \; , \tag{39}$$

where $\chi(x)$ is the Thomas-Fermi function, well known and tabulated, of the scaling variable $x = 2(4/3\pi)^{2/3} m\alpha Z^{1/3}$, the energy scale T_0 is given by

$$T_0 = 2 \left(\frac{4}{3\pi}\right)^{2/3} m\,\alpha^2\, Z^{4/3} \approx 30.8\, Z^{4/3}\, \text{eV} \; , \tag{40}$$

and, finally, $x_0(T)$ is the point where the integrand becomes zero, i.e. corresponding to the radius beyond which all the electrons are active at the given energy T. The energy scale T_0 in germanium (Z=32) evaluates to $T_0 \approx 3.1\,\text{keV}$. The Thomas-Fermi activation factor for germanium calculated from the formula (39) is shown by the dashed line in the plot of Fig. 2. One can see that in the shown energy range it reasonably approximates the stepping behavior of the atomic orbitals. The discussed statistical model is known to approximate the average bulk properties of the atomic electrons with a relative accuracy $O(Z^{-2/3})$ and as long as the essential distances r satisfy the condition $Z^{-1} \ll m\alpha r \ll 1$, which condition in terms of the scaling variable x reads as $Z^{-2/3} \ll x \ll Z^{1/3}$. In terms of the formula (39) for the number of active electrons, the lower bound on the applicability of the model is formally broken at $T \sim Z^{2/3} T_0$, i.e. at the energy scale of the inner atomic shells. However the effect of the deactivation of the inner electrons is small, of order Z^{-1} in comparison with the total number Z of the electrons. On the other hand, at low T, including the most interesting region of $T \sim T_0$, the integral in Eq.(39) is determined by the range of x of order one, where the model treatment is reasonably justified.

In order to apply the same model for an estimate of the correlation effect we replace in the estimated correlation contribution to the magnetic neutrino scattering in Eq.(38) the factor $|\psi(0)|^2$ by the total density of the electrons that an active electron 'sees' at its location in the atom. Then the resulting correction to the integral I_1 for an atom can be written in terms of the density $n_a(r)$ of the active electrons and the total density $n(r)$ of the electrons in the atom:

$$I_{1c} = -\frac{\pi\,\alpha}{2\,m\,T^3} \int n_a(r)\,n(r)\,d^3r. \tag{41}$$
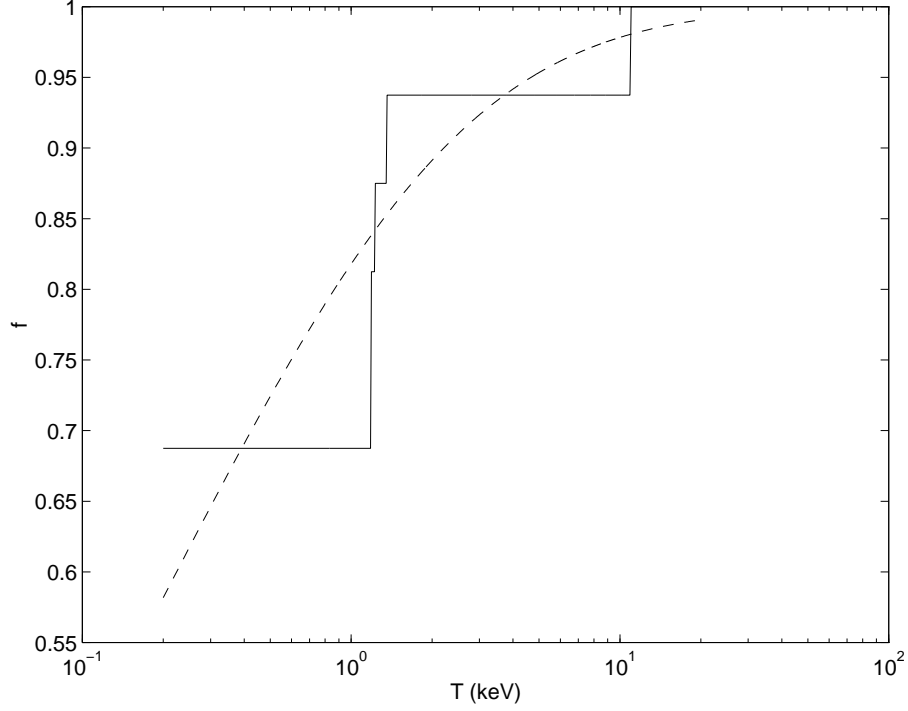
FIG. 2: The activation factor f for germanium in the stepping approximation with the actual energies of the orbitals (solid line) and its interpolation in the Thomas-Fermi model (dashed).

It should be pointed out that the numerical coefficient in this expression contains a factor of $1/8$ as compared to Eq.(38). This is because of a factor of $1/4$ corresponding to the statistical weight of the spin-singlet state and an extra $1/2$ compensating for the double counting of electrons in the pairs.

One can write the correction described by Eq.(41) in terms of a correction to the activation factor in the Thomas-Fermi model as

$$
\begin{aligned}
f_c(T) &\equiv T\,\frac{I_{1c}}{Z} = \\
&-\left(\frac{T_1}{T}\right)^2 \left\{ \int_{x(T)}^{\infty} \chi^3(x)\,\frac{dx}{x} + \int_0^{x(T)} \chi^{3/2}(x) \left[\chi^{3/2}(x) - \left(\chi(x) - \frac{T}{T_0}x\right)^{3/2}\right] \frac{dx}{x} \right\}
\end{aligned} \tag{42}
$$

where the correlation energy scale T_1 is given by

$$
T_1 = \frac{\sqrt{2}}{3\pi}\, m\,\alpha^2\,Z \approx 4.1\,Z\,\mathrm{eV} \tag{43}
$$

and evaluates to about $131\,\mathrm{eV}$ in germanium. The plot of the estimated correlation correction in germanium is shown in Fig. 3. One can readily see that this correction is below 1.5% at

16

$T \approx 0.3\,\text{keV}$ and rapidly decreases at higher energy transfer. Clearly, this estimate refers only to the magnetic part of the scattering, while for the weak part we find no correlation effect in the considered order due to the cancellation found in Eq.(38). We thus conclude that in the range of values of T above a few hundred eV the correlation effect can be safely neglected for both contributions to the neutrino scattering on germanium.
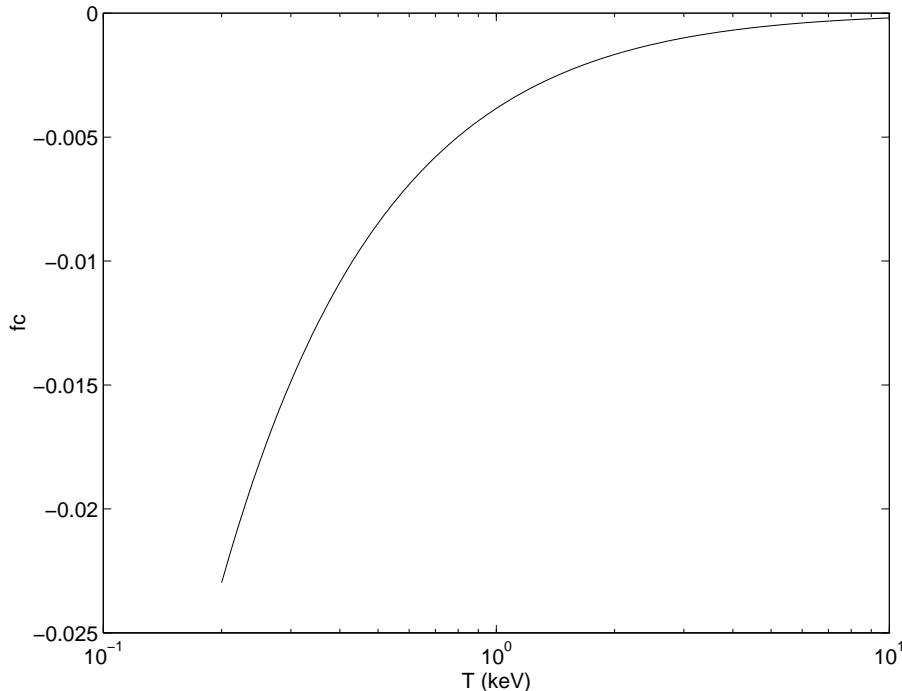

FIG. 3: The correlation correction f_c to the activation factor f for germanium in the Thomas-Fermi model.

VI. SUMMARY

We have considered the scattering of neutrinos on electrons bound in atoms. Our main finding is that the differential over the energy transfer cross section given by the free-electron formulas (1) and (2) and the stepping behavior of the activation factor given by Eq.(21) provides a very accurate description of the neutrino-impact ionization of a complex atom, such as germanium, down to quite low energy transfer. The deviation from this approximation due to the onset of the ionization near the threshold is less than 5% (of the height of the

step) for the K electrons, if one applies the analytical behavior of this onset that we find for the ground state of a hydrogen-like ion. We also find that the free-electron expressions for the cross section are not affected by the atomic binding effects in the semiclassical limit and for independent electrons. For this reason we expect that the deviation of the actual onset from a step function at the threshold for ionization of higher atomic orbitals is even smaller than for the ground state, since the motion in the higher states is closer to the semiclassical limit. The approximation of independent electrons lacks an account for the two-electron correlations arising from the Coulomb interaction between the electrons in the atom. We estimate this effect in the large Z limit using the Thomas-Fermi model and argue that the effect of the correlations is small in germanium for the values of the energy transfer above $0.2 \div 0.3\,\mathrm{keV}$. We thus argue that for practical applications, i.e. for the analysis of data of the searches for NMM one can safely apply the free-electron formulas and the stepping approximation at the energy transfer down to this range.

Acknowledgments

Appendix A: Sum rules

We consider here the general sum rules for the dynamical structure factor $S(T, q^2)$, which stem from the analyticity of the density-density Green's function $F(T, q^2)$ at a fixed T and complex q^2 and also from its asymptotic behavior at large large $|q^2|$. At a non zero T the dynamical structure function, defined by Eq.(6), vanishes at $q^2 = 0$, due to the orthogonality of the excited states $|n\rangle$ and the initial state $|0\rangle$ in Eq.(6) since $\rho(0)$ reduces to a unit operator. For this reason the function $F(T, q^2)$ is real at $q^2 = 0$ and thus satisfies in the complex plane the condition $F(T, z^*) = F^*(T, z)$. At a non zero real q^2 the imaginary part of this function is not vanishing for both positive and *negative* q^2, so that it has cuts along the real axis extending from zero to both infinities [22]. On the other hand, the asymptotic at large $|q^2|$ behavior of the Green's function $F(T, q^2)$ is determined by the free-electron formula (16), since at $|q^2| \to \infty$ any interaction terms can be neglected. For a scattering on an atom with

Z electrons one finds

$$F(T, q^2)\big|_{|q^2|\to\infty} \to -\frac{2m\,Z}{q^2} \ . \tag{A1}$$

This behavior enables one to write a dispersion relation for the Green's function with no subtractions:

$$F(T, q^2) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{Im}F(T, Q^2)}{Q^2 - q^2 - i\epsilon}\, dQ^2 \ . \tag{A2}$$

By comparing the dispersion relation at $q^2 \to \infty$ with the asymptotic behavior in Eq.(A1) one readily finds the sum rule for an integral similar to I_2, but extended to include also the negative q^2:

$$\int_{-\infty}^{\infty} S(T, q^2)\, dq^2 = 2m\,Z \ , \tag{A3}$$

where the dynamical structure function at negative q^2 is defined by the analytical continuation and Eq.(10), rather than by Eq.(6).

In order to derive from Eq.(A2) a relation for an integral similar to I_1 it is necessary to consider the Green's function near the origin, i.e. at $q^2 \to 0$. In multi-electron systems the behavior in this region is generally complicated by the two-electron correlations. For this reason we limit the consideration here to the system with just one electron, $Z = 1$. In such a system one has $\rho(\vec{q}) \to 1$ at $q \to 0$, so that the Green's function in Eq.(8) is contributed by only the initial state $|0\rangle$:

$$F(T, 0) = \frac{1}{T} \ . \tag{A4}$$

By comparing this formula with Eq.(A2) at $Q^2 \to 0$ one immediately finds the sum rule

$$\int_{-\infty}^{\infty} S(T, q^2)\, \frac{dq^2}{q^2} = \frac{1}{T} \ . \tag{A5}$$

It should be pointed out that unlike the sum rule (A3) this latter relation is generally invalidated in multi-electron system by the correlation effects. In fact an indication of such a difference in the behavior of the two integrals can be seen in Eq.(38), where the discussed there correlation effect vanishes for the integral I_2, but not for the I_1.

The sum rule (A5) can also be derived from the latter expression in Eq.(18). Indeed one can rewrite the formula as

$$F(T, q^2) = \frac{1}{T - \frac{q^2}{2m}} + \frac{1}{T - \frac{q^2}{2m}} \left\langle 0 \left| \frac{1}{T - \frac{q^2}{2m} - \frac{(\vec{p}\cdot\vec{q})}{m} - H + E_0}\, \frac{(\vec{p}\cdot\vec{q})}{m} \right| 0 \right\rangle \ , \tag{A6}$$

and consider the expansion of the last term in powers of $(\vec{p}\cdot\vec{q})$. Only the even terms in this expansion are non vanishing, since the odd terms give zero due to the parity. One can

19

readily see that in each term in the expansion the pole in q^2 is of a higher order than the power of q^2 in the numerator, so that the imaginary part of each term integrates to zero in the integral as in Eq.(A5), while the term of the zeroth order in $(\vec{p} \cdot \vec{q})$ in Eq.(A6) gives the sum rule (A5). It is again important here that the integration runs over all values of q^2 i.e. from $-\infty$ to $+\infty$, since only in this case all the poles of the terms in the expansion are within the integration range. Any restriction of the range of integration over q^2 may leave some poles out so that the vanishing of the contribution of all higher terms in the expansion is generally not guaranteed.

Appendix B: Momentum-transfer integrals for hydrogen-like states

Consider the situation when the initial electron occupies the discrete nl orbital in a Coulomb potential $V(\vec{r}) = -\alpha Z/r$. The dynamical structure factor for this hydrogen-like system is given by

$$S_{(nl)}(T, q^2) = \frac{mk}{(2\pi)^3} \frac{1}{2l+1} \sum_{m_l=-l}^{l} \int d\Omega_k |\langle \varphi_{\vec{k}}^- | \rho(\vec{q}) | \varphi_{nlm_l} \rangle|^2, \tag{B1}$$

where φ_{nlm_l} is the bound-state wave function, $\varphi_{\vec{k}}^-$ is the outgoing Coulomb wave for the ejected electron with momentum $\vec{k}$, and $k = |\vec{k}| = \sqrt{2mT - p_n^2}$, with $p_n = \alpha Z m/n$ being the electron momentum in the nth Bohr orbit. The closed-form expressions for the bound-free transition matrix elements in Eq. (B1) can be found, for instance, in Ref. [16]. In principle, they allow for performing angular integrations in Eq. (B1) analytically. This task, however, turns out to be formidable for large values of n. Therefore, below we restrict our consideration to the $n = 1, 2$ states only, which nevertheless is enough for demonstrating the validity of the semiclassical approach developed in Sec. III.

Using results of Ref. [17], we can present the function (B1) when $n = 1, 2$ as

$$S_{(nl)}(T, q^2) = \frac{2^8 m p_n^6}{3[1 - \exp(-2\pi\eta)]} \frac{q^2 f_{nl}(q^2)}{[(q^2 - k^2 + p_n^2)^2 + 4p_n^2 k^2]^{2n+1}}$$
$$\times \exp\left[-2\eta \arctan\left(\frac{2p_n k}{q^2 - k^2 + p_n^2}\right)\right], \tag{B2}$$

where the branch of the arctangent function should be used that lies between 0 and π,

$\eta = \alpha Z m / k$ is the Sommerfeld parameter, and

$$f_{1s}(q^2) = 3q^2 + k^2 + p_1^2, \tag{B3}$$

$$
\begin{aligned}
f_{2s}(q^2) = {} & 8 \Big[3q^{10} - (32p_2^2 + 11k^2)q^8 + (82p_2^4 + 72p_2^2 k^2 + 14k^2)q^6 \\
& + (20p_2^6 - 62p_2^4 k^2 - 20p_2^2 k^4 - 6k^6)q^4 + (p_2^2 + k^2) \\
& \times \left(\frac{47}{5}p_2^6 - \frac{47}{5}p_2^4 k^2 - 7p_2^2 k^4 - k^6 \right) q^2 + (4p_2^2 + k^2)(p_2^2 + k^2)^4 \Big],
\end{aligned} \tag{B4}
$$

$$
\begin{aligned}
f_{2p}(q^2) = {} & 2p_2^2 \Big[36q^8 - 48(p_2^2 + k^2)q^6 + (152p_2^4 - 48p_2^2 k^2 - 8k^4)q^4 + (p_2^2 + k^2) \\
& \times \left(\frac{1712}{15}p_2^4 + \frac{1568}{15}p_2^2 k^2 + 16k^4 \right) q^2 + \left(\frac{44}{3}p_2^2 + 4k^2 \right)(p_2^2 + k^2)^3 \Big].
\end{aligned} \tag{B5}
$$

Insertion of Eq. (B2) into the integrals (15) and integration over q^2, using the change of variable

$$\frac{2p_n k}{q^2 - k^2 + p_n^2} = \tan x$$

and the standard integrals involving the products of the exponential function and the powers of sine and cosine functions, yields

$$
\begin{aligned}
I_1^{(1s)}(T) = \frac{I_2^{(1s)}(T)}{2mT} = {} & \frac{T^{-1}}{1 - \exp(-\frac{2\pi}{\sqrt{y_1 - 1}})} \left\{ 1 - \exp\left(-\frac{\pi}{\sqrt{y_1 - 1}} \right) \right. \\
& \left. \times \exp\left[\frac{-2}{\sqrt{y_1 - 1}} \arctan\left(\frac{y_1 - 2}{2\sqrt{y_1 - 1}} \right) \right] \left(1 - \frac{4}{y_1} + \frac{16}{3y_1^2} \right) \right\},
\end{aligned} \tag{B6}
$$

$$
\begin{aligned}
I_1^{(2s)}(T) = {} & \frac{T^{-1}}{1 - \exp(-\frac{4\pi}{\sqrt{y_2 - 1}})} \left\{ 1 - \exp\left(-\frac{2\pi}{\sqrt{y_2 - 1}} \right) \right. \\
& \left. \times \exp\left[\frac{-4}{\sqrt{y_2 - 1}} \arctan\left(\frac{y_2 - 2}{2\sqrt{y_2 - 1}} \right) \right] \left(1 - \frac{8}{y_2} + \frac{80}{3y_2^2} - \frac{448}{15y_2^3} + \frac{1792}{15y_2^4} \right) \right\},
\end{aligned} \tag{B7}
$$

$$
\begin{aligned}
I_2^{(2s)}(T) = {} & \frac{2m}{1 - \exp(-\frac{4\pi}{\sqrt{y_2 - 1}})} \left\{ 1 - \exp\left(-\frac{2\pi}{\sqrt{y_2 - 1}} \right) \right. \\
& \left. \times \exp\left[\frac{-4}{\sqrt{y_2 - 1}} \arctan\left(\frac{y_2 - 2}{2\sqrt{y_2 - 1}} \right) \right] \left(1 - \frac{8}{y_2} + \frac{80}{3y_2^2} - \frac{448}{15y_2^3} + \frac{1024}{15y_2^4} \right) \right\},
\end{aligned} \tag{B8}
$$

$$
\begin{aligned}
I_1^{(2p)}(T) = {} & \frac{T^{-1}}{1 - \exp(-\frac{4\pi}{\sqrt{y_2 - 1}})} \left\{ 1 - \exp\left(-\frac{2\pi}{\sqrt{y_2 - 1}} \right) \right. \\
& \left. \times \exp\left[\frac{-4}{\sqrt{y_2 - 1}} \arctan\left(\frac{y_2 - 2}{2\sqrt{y_2 - 1}} \right) \right] \left(1 - \frac{8}{y_2} + \frac{80}{3y_2^2} - \frac{704}{15y_2^3} + \frac{3328}{45y_2^4} \right) \right\},
\end{aligned} \tag{B9}
$$

$$I_2^{(2p)}(T) = \frac{2m}{1 - \exp(-\frac{4\pi}{\sqrt{y_2-1}})} \left\{ 1 - \exp\left(-\frac{2\pi}{\sqrt{y_2-1}}\right) \right.$$
$$\left. \times \exp\left[\frac{-4}{\sqrt{y_2-1}} \arctan\left(\frac{y_2-2}{2\sqrt{y_2-1}}\right)\right] \left(1 - \frac{8}{y_2} + \frac{80}{3y_2^2} - \frac{704}{15y_2^3} + \frac{512}{15y_2^4}\right) \right\},$$

$$(B10)$$

where $y_n = 2mT/p_n^2 \equiv T/|E_n|$. The largest deviations of these integrals from the free-electron analogs (17) occur at the ionization threshold $T = |E_n|$. The corresponding relative values in this specific case are

$$\frac{I_1^{(1s)}}{I_1^{(FE)}} = \frac{I_2^{(1s)}}{I_2^{(FE)}} = 1 - \frac{7}{3}e^{-4} = 0.9572635093,$$

$$\frac{I_1^{(2s)}}{I_1^{(FE)}} = 1 - \frac{1639}{15}e^{-8} = 0.9633451168, \qquad \frac{I_2^{(2s)}}{I_2^{(FE)}} = 1 - \frac{871}{15}e^{-8} = 0.9805208034,$$

$$\frac{I_1^{(2p)}}{I_1^{(FE)}} = 1 - \frac{2101}{45}e^{-8} = 0.9843376226, \qquad \frac{I_2^{(2p)}}{I_2^{(FE)}} = 1 - \frac{103}{15}e^{-8} = 0.9976964900.$$

The above results indicate a clear tendency: the larger n and l, the closer $I_1^{(nl)}$ and $I_2^{(nl)}$ are to the free-electron values. The departure from the free-electron behavior does not exceed several percent at most. These observations provide a solid base for the semiclassical approach of Sec. III.

---

[1] K. Fujikawa and R. Shrock, Phys. Rev. Lett. **45**, 963 (1980).

[2] C. Giunti and A. Studenikin, Phys. Atom. Nucl. **72**, 2089 (2009) [arXiv:0812.3646 [hep-ph]].

[3] H. T. Wong *et al.* [TEXONO Collaboration], Phys. Rev. D **75**, 012001 (2007) [arXiv:hep-ex/0605006].

[4] A. G. Beda *et al.*, Phys. Atom. Nucl. **70**, 1873 (2007) [arXiv:0705.4576 [hep-ex]].

[5] A. G. Beda *et al.*, arXiv:1005.2736 [hep-ex].

[6] G. V. Domogatskii and D. K. Nadezhin, Sov. J. Nucl. Phys. **12**, 678 (1971)

[7] P. Vogel and J. Engel, Phys. Rev. D **39**, 3378 (1989).

[8] V. I. Kopeikin, L. A. Mikaelyan, V. V. Sinev and S. A. Fayans, Yad. Fiz. **60**, 2032 (1997).

[9] S. A. Fayans, L. A. Mikaelyan and V. V. Sinev, Phys. Atom. Nucl. **64**, 1475 (2000) [Yad. Fiz. **64**, 1551 (2000); arXiv:hep-ph/0004158]

[10] H. T. Wong, H. B. Li and S. T. Lin, Phys. Rev. Lett. **105**, 061801 (2010) [arXiv:1001.2074v2 [hep-ph]].

[11] M. B. Voloshin, Phys. Rev. Lett. **105**, 201801 (2010) [arXiv:1008.2171 [hep-ph]].

[12] H. T. Wong, H. B. Li and S. T. Lin, arXiv:1001.2074v3 [hep-ph], November 2010.

[13] K. A. Kouzakov and A. I. Studenikin, Phys. Lett. B **696**, 252 (2011) [arXiv:1011.5847 [hep-ph]].

[14] L. D. Landau and E. M. Lifshits, *Quantum Mechanics (Non-relativistic Theory)*, Third Edition, Pergamon, Oxford, 1977.

[15] L. Van Hove, Phys. Rev. **95**, 249 (1954).

[16] Dž. Belkić, J. Phys. B: At. Mol. Phys. **14**, 1907 (1981).

[17] A. R. Holt, J. Phys. B: At. Mol. Phys. **2**, 1209 (1969).

[18] The sum rules of Appendix A correct the omissions made in Ref. [11]

[19] It can be also noted that both integrals are modified in exactly the same proportion, so that their ratio is not affected at any T: $I_2(T)/I_1(T) = 2mT$. We find however that this exact proportionality is specific for the ionization from the ground state in the Coulomb potential.

[20] The appearance of the free-electron expressions here is not surprising, since the equation (19) can be also viewed as the one for scattering on an electron boosted to the momentum p

[21] Indeed one has $|F| = \alpha/r^2 \sim m^2 \alpha^3 n^4$ and $p \sim m\alpha/n$, so that $m|F|/p^3 \sim 1/n$.

[22] It is not clear what physical meaning can be ascribed in this problem to negative q^2. However a formal analytical continuation to negative q^2 exists and results in a cut along the negative real axis. It is the omission of this cut that resulted in a somewhat incorrect treatment of the problem in Ref. [11].